Finite-range effects in dilute Fermi gases at unitarity

Stefano Simonucci*[a,b], Giovanni Garberoglio[b], Simone Taioli[b,c]
[a] Department of Physics, University of Camerino, via Madonna delle Carceri 9, 62032 Camerino, Italy - INFN Sezione Perugia
[b] Interdisciplinary Laboratory for Computational Science (LISC), FBK-CMM and University of Trento, via Sommarive 18, I-38123 Trento, Italy
[c] Department of Physics, University of Trento, Via Sommarive 14, I-38123, Trento, Italy
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We develop a theoretical method going beyond the contact-interaction approximation frequently used in mean-field theories of many-fermion systems, based on the low-energy T-matrix of the pair potential to rigorously define the effective radius of the interaction. One of the main consequences of our approach is the possibility to investigate finite-density effects, which are outside the range of validity of approximations based on δ-like potentials. We apply our method to the calculation of density dependent properties of an ultracold gas of ^{6}Li atoms at unitarity, whose two-body interaction potential is calculated using *ab initio* quantum chemistry methods. We find that density effects will be significant in ultracold gases with densities one order of magnitude higher than those attained in current experiments.

I. INTRODUCTION

In recent years, remarkable experimental advances in the field of trapped alkali gases made it possible to tune the interaction of fermionic atoms and study experimentally the transition between a BCS state of paired fermions to a BEC state of diatomic molecules [1].

Several interesting phenomena occurring in these and other fermionic systems are usually analyzed by using a mean-field treatment of a model short-range fermion-fermion interaction, broadly assumed to be a contact potential depending only on the s-wave scattering length a of the form

$$\hat{V}(\mathbf{r}) = \frac{4\pi a}{m}\delta(\mathbf{r}). \tag{1}$$

This model potential, known as Fermi Contact Interaction (FCI), has been used for calculating, for example, the weak interaction in nucleon systems [2] and for describing the Darwin correction in the theory of hydrogen-like atoms [3].

FCI has been used successfully to describe Fermi systems (cold atomic gases and nuclear matter in particular) in the mean-field approximation, that is within the framework of the Bogoliubov–de Gennes (BdG) equations [1, 4–7]. However, the self-consistent solution of the BdG gap equation using FCI with an external potential diverges, leading to an infinite pairing [8]. This divergence can be renormalized as shown in Refs. [8–10], even in the experimentally and theoretically relevant unitary limit ($a \to \infty$) [11–13], where the behavior of a fermionic system displays universal properties. However, in this latter case, the Hartree–Fock (HF) term appearing in the BdG equations diverges as well, but this divergence is usually neglected [1, 6].

Recently, few research groups have investigated the effect of the finite-range of the potential on the properties of dilute Fermi systems, therefore going beyond the FCI description. In these approaches the authors introduce an effective interatomic potential characterized by two length scales which allow to fix independently the scattering length and the potential range [14–16]. Previous efforts to calculate the energy spectrum of non ideal Fermi [17] and Bose [18] gases with short range potentials have been limited to small densities by using perturbative expansion to the second order in the parameter $k_F f_0$, where f_0 is the scattering amplitude, within Green's function formalism. The importance of ultracold ^{6}Li gas in the unitary regime goes beyond the milestone experiment on superfluid pairing by Ketterle [19] as it represents a prototype of other strongly interacting fermions, such as neutron matter [20] and dense quark matter [21].

In this paper, we show how to include density effects in a mean-field description of dilute Fermi gases. We achieve this goal by using the on-shell T matrix of the pair-potential as the appropriate description of the interactions and of their effective range. We will show that this approach removes the unphysical divergences obtained with a δ-like potential, and allows us to investigate – in a mean field approximation – density effects in various observable quantities characterizing dilute Fermi gases. As a case-study, we solve the BdG equations [4, 22] for a homogeneous system of ^{6}Li atoms in the unitary regime, focusing on the definition of the effective radius of the multichannel scattering potential, obtained from *ab-initio* calculations. At variance with approaches based on the momentum expansion of the s-wave phase shift, our theory predicts the same value of the potential range for both of the Feshbach resonances present in this system.

This paper is organized as follows: in Sec. II we derive the principal equations. We present our approach where the contact potential is seen as a limit of separable potentials, and the BdG equations are written in terms of the T-matrix. This formalism is applied to ^{6}Li in Sec. III, where we also describe how we obtained the interatomic potential using *ab-initio* calculations. The results regarding finite-range effects in this system are reported in Sec. IV.

II. THE T-MATRIX AS THE BASIC BUILDING BLOCK OF BDG

A. The contact potential as a limit of separable potentials

In general terms, one can write a two-body interaction potential as

$$\hat{V} = \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}'_1 d\mathbf{r}'_2 \ \psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2) \times V(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}'_1, \mathbf{r}'_2)\psi(\mathbf{r}'_2)\psi(\mathbf{r}'_1) \quad (2)$$

where $\psi^\dagger(\mathbf{r})$ is the creation operator of a particle at position $\mathbf{r}$. If, the interaction is translationally invariant, then the matrix elements in the previous equation factorize as:

$$V(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}'_1, \mathbf{r}'_2) = v(\mathbf{r}_1 - \mathbf{r}_2; \mathbf{r}'_1 - \mathbf{r}'_2) \times \delta\left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} - \frac{\mathbf{r}'_1 + \mathbf{r}'_2}{2}\right). \quad (3)$$

Furthermore, a *local* potential is characterized by the condition

$$v(\mathbf{r}; \mathbf{r}') = \phi(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}'), \quad (4)$$

where $\phi(\mathbf{r})$ is the diagonal part of the potential and we have defined $\mathbf{r} = \mathbf{r_1} - \mathbf{r_2}$ and $\mathbf{r}' = \mathbf{r}'_\mathbf{1} - \mathbf{r}'_\mathbf{2}$. We call a potential *separable* if there exists a function $f(\mathbf{r})$ so that

$$v(\mathbf{r}; \mathbf{r}') = f(\mathbf{r})f(\mathbf{r}'). \quad (5)$$

From the above definition sit is clear that the contact potential is both local and separable. In the usual renormalization schemes, FCI is obtained as the $n \to \infty$ limit of a a series of local potentials $\phi_n(\mathbf{r})$. In this paper we take the complementary route and define the contact potential as a limit of separable potentials $f_n(\mathbf{r})$. In our approach the contact potential is seen as the limit of a series of projectors onto a uni-dimensional manifold. Therefore we write it as a limit of separable potentials with progressively small radius:

$$V(\mathbf{r}, \mathbf{r}') = \lim_{n\to\infty} f_n(\mathbf{r}) V_n f_n^*(\mathbf{r}') \quad (6)$$

where V_n is a term of this sequence (to be specified below) and $f_n(\mathbf{r})$ is defined in term of a normalized arbitrary function $f(\mathbf{r})$ such that $f_n(\mathbf{r}) = \sqrt{n^3} f(n\mathbf{r})$. Our idea is to find the sequence V_n so that the T-matrix corresponding to the potential in Eq. (6) describes the proper scattering length a of the system. In doing so we will exploit the properties of the on-shell T-matrix at zero energy. Its fundamental role in our approach is further made clear by identifying the radius of the effective range of the interactions using the expansion of the on-shell T-matrix at zero momentum. This definition of the effective range differs from the usual one, which is based on the value of the first order correction to the s-wave phase shift [23]

$$k \ \cot\delta_0 = -\frac{1}{a} + \frac{1}{2}a_0 k^2 + \cdots \quad (7)$$

In our approach we expand the on-shell T-matrix at zero energy, $T_+(0)$, around $\mathbf{k} = 0$ obtaining:

$$T_+(0; \mathbf{k}, \mathbf{k}') \simeq \frac{4\pi a}{m} - c(k^2 + k'^2). \quad (8)$$

For $\mathbf{k}, \mathbf{k}' \approx 0$, c is related to the range of the on-shell $T_+(0)$ matrix in the $\mathbf{k}$-space or, by Fourier-transform, to the inverse of the range of the $T_+(0)$ in the configuration space. Therefore, we define the effective range of the potential as:

$$r_0 = \sqrt{\frac{cm}{\pi|a|}}. \quad (9)$$

In order to specify the sequence V_n appearing in Eq. (6) we remind that the scattering length is related to the on-shell T-matrix via the equation:

$$\frac{4\pi a}{m} = \lim_{k\to 0} \langle k|T_+|k\rangle \quad (10)$$

and that the Lippmann–Schwinger (LS) equation $T = V + VG_0(E)T$ can be written as

$$T(E) = \frac{1}{V^{-1} - G_0(E)}, \quad (11)$$

where $G_0(E)$ is the free-particle Green's function at energy E. Expanding $G_0(E)$ in the momentum space one obtains:

$$\langle f|\frac{1}{E - K + i\varepsilon}|f\rangle = Q_0 + iQ_1 k + \frac{1}{2}Q_2 k^2 + \cdots \quad (12)$$

where K is the kinetic energy, $E = \frac{k^2}{m}$, and it can be shown that $Q_1 = -m|\langle k = 0|f\rangle|^2/(4\pi)$. In terms of the elements of the sequence f_n defined above, one has:

$$\langle f_n|\frac{1}{E - K + i\varepsilon}|f_n\rangle = \frac{1}{n^2}\langle f|\frac{1}{\frac{E}{n^2} - K + i\varepsilon}|f\rangle = \frac{Q_0}{n^2} + iQ_1\frac{k}{n^3} + \frac{1}{2}Q_2\frac{k^2}{n^4} + \cdots \quad (13)$$

and therefore Eq. (11) becomes

$$\langle \mathbf{k}|T_{n+}|\mathbf{k}'\rangle = = \frac{\langle \mathbf{k}/n|f\rangle\langle f|\mathbf{k}'/n\rangle/n^3}{\left(\frac{1}{V_n} - \frac{Q_0}{n^2} - iQ_1\frac{k}{n^3} - \frac{1}{2}Q_2\frac{k^2}{n^4} - \cdots\right)} \quad (14)$$

By choosing

$$V_n = \frac{n^2}{Q_0 + \frac{Q_1}{an}} \quad (15)$$

one obtains the correct scattering length in the limit $n \to \infty$ since, for $\mathbf{k}, \mathbf{k}' \approx 0$:

$$\lim_{n\to\infty}\langle \mathbf{k}|T_{n+}(0)|\mathbf{k}'\rangle = \frac{1}{n^3}\frac{\langle \mathbf{k}/n|f\rangle\langle f|\mathbf{k}'/n\rangle}{1/V_n - Q_0/n^2} = \frac{4\pi a}{m} \quad (16)$$

With the same choice, the limiting value of the matrix elements of the potential are:

$$\langle \mathbf{k}|V|\mathbf{k}'\rangle = \lim_{n\to\infty}\langle \mathbf{k}|f_n\rangle V_n\langle f_n|\mathbf{k}'\rangle = \lim_{n\to\infty}\frac{\langle \mathbf{k}|f_n\rangle\ n^2\ \langle f_n|\mathbf{k}'\rangle}{Q_0+\frac{Q_1}{an}} = \lim_{n\to\infty}\frac{1}{n^3}\frac{\langle \mathbf{k}/n|f\rangle\ n^2\ \langle f|\mathbf{k}'/n\rangle}{Q_0+\frac{Q_1}{an}} = 0. \quad (17)$$

Therefore, within our approach $T_+(0)$ is a δ function for regular functions and has a different behavior for not regular ones. At variance with Huang pseudo-potential, for any $g(\mathbf{r})\sim 1/r$ at the origin one obtains, by using the definition in Eq. (15):

$$\lim_{n\to\infty}\langle \mathbf{k}|V_n|g\rangle = \lim_{n\to\infty}\frac{1}{n^3}\frac{\langle \mathbf{k}/n|f\rangle\ n^3\langle f|g\rangle}{Q_0+\frac{Q_1}{an}} = \frac{\langle 0|f\rangle\langle f|g\rangle}{Q_0} \quad (18)$$

while, as by Eq. (17), for regular functions the potential matrix elements are zero.

Notice that, from Eqs. (6), (10), and (11) we have, denoting by $|0\rangle$ the zero-momentum state and setting $g_n=\langle f_n|G_0|f_n\rangle$,

$$\frac{4\pi a}{m} = \lim_{n\to\infty}\langle 0|f_n\rangle\frac{1}{n^3\left(V_n^{-1}-g_n\right)}\langle f_n|0\rangle. \quad (19)$$

In the $n\to\infty$ limit, the sequence of $\sqrt{n^3}\langle x|f_n\rangle$ is proportional to the δ function, and the matrix element $n^3 g_n$ tends to infinity. As a consequence, one has

$$\lim_{n\to\infty}\frac{V_n}{n^3}=0. \quad (20)$$

B. The Bogoliubov–de Gennes equations for a separable potential

The Hamiltonian of a system of fermions in an external potential $\hat{U}(x)$ and interacting with a two-body potential $\hat{V}$ is, in the second quantized formalism,

$$H=\sum_{ij}\left(T_{ij}+U_{ij}\right)\ a_i^\dagger a_j+\frac{1}{2}\sum_{il,jm}V_{il,jm}\ a_i^\dagger a_l^\dagger a_m a_j, \quad (21)$$

where $a_i^\dagger$ and a_i are the creation and annihilation operators for a complete set of single particle states. The indices of these operators describe all the relevant quantum numbers.

A mean-field solution of the ground state of the Hamiltonian (21) can be obtained by introducing an effective Hamiltonian $H_{\rm eff}$, where the two-body potential V in Eq. (21) is substituted by an effective one-body potential

$$V_{\rm eff}=\sum_{ij}\left(W_{ij}\ a_i^\dagger a_j+\frac{1}{2}\Delta_{ij}^*\ a_i a_j+\frac{1}{2}\Delta_{ij}\ a_i^\dagger a_j^\dagger\right), \quad (22)$$

where the as-yet unspecified matrices W_{ij} and Δ_{ij} are determined by requiring that the average values of H and $H_{\rm eff}-\mu\hat{N}$ are as close as possible to each other. In the evaluation of the average value of H, one uses the Hartree–Fock–Gorkov (HFG) factorization of the two-body density matrix which, in the case of fermions, is [24]

$$\langle a_i^\dagger a_l^\dagger a_m a_j\rangle = \langle a_i^\dagger a_j\rangle\langle a_l^\dagger a_m\rangle - \langle a_i^\dagger a_m\rangle\langle a_l^\dagger a_j\rangle + \langle a_i^\dagger a_l^\dagger\rangle\langle a_j a_m\rangle. \quad (23)$$

The self-consistent equations for W_{ij} and Δ_{ij} turn out to be:

$$W_{ij}=\sum_{l,m}\left(V_{il,jm}-V_{il,mj}\right)\ \langle a_l^\dagger a_m\rangle \quad (24)$$

$$\Delta_{ij}=-\sum_{l,m}V_{ij,lm}\ \langle a_l a_m\rangle, \quad (25)$$

and one is left with a two-body effective Hamiltonian, which can be put in the form

$$H_{\rm eff}=\sum_k \epsilon_k\ b_k^\dagger b_k+E_0, \quad (26)$$

where E_0 is the ground state energy. The sum over k is restricted to those states where $\epsilon_k\geq 0$. The new set of fermionic operators b_k and $b_k^\dagger$ are given by the Bogoliubov transform

$$\begin{aligned} a_i &= \sum_j\left(u_{ij}b_j+v_{ij}^* b_j^\dagger\right)\\ a_i^\dagger &= \sum_j\left(u_{ij}^* b_j^\dagger+v_{ij}b_j\right), \end{aligned} \quad (27)$$

and satisfy the relation

$$\langle b_i^\dagger b_j\rangle = \frac{\delta_{ij}}{\exp\left(\frac{\epsilon_i}{k_B T}\right)+1}, \quad (28)$$

although in the following we will be concerned, for the sake of conciseness, with the $T\to 0$ limit.

The equations determining the coefficients u_{ij} and v_{ij} appearing in equation (27) are the well known Bogoliubov–de Gennes equations [4]:

$$\begin{aligned} \sum_k\left[\left(T_{ik}+U_{ik}+W_{ik}-\mu\delta_{ik}\right)u_{kj}+\Delta_{ik}v_{kj}\right] &= \epsilon_j u_{ij},\\ \sum_k\left[\left(T_{ik}+U_{ik}+W_{ik}+\mu\delta_{ik}\right)^* v_{kj}+\Delta_{ik}^* u_{kj}\right] &= -\epsilon_j v_{ij}, \end{aligned} \quad (29)$$

which have to be solved self-consistently with the definitions of W_{ij} and Δ_{ij} given in equations (24) and (25), respectively.

In our approach, where the FCI is seen as a limit of separable potentials, the HF term of Eq. (24) turns out to be zero. In order to see that, we remind that the Latin indices in the previous equations were a short-hand notation to indicate both spin and spatial degrees of freedom. For example, one has

$$\langle a_l^\dagger a_m\rangle = \varrho_{\alpha\beta}(\mathbf{r},\mathbf{r}') = \sum_\eta\int d\mathbf{x}\ v_{\alpha\eta}(\mathbf{r},\mathbf{x})v_{\beta\eta}^*(\mathbf{r}',\mathbf{x}) \quad (30)$$

where $\varrho_{\alpha\beta}(\mathbf{r},\mathbf{r}')$ is the one-body density matrix, with the Greek letters indicating spin degrees of freedom. If we further assume that the pair potential is given by

$$V_{ij,lm} = \delta_{\alpha\gamma}\delta_{\beta\delta} f_n(\mathbf{R}-\mathbf{R}') V_n f_n(\mathbf{r}-\mathbf{r}')\delta\left(\frac{\mathbf{r}+\mathbf{r}'}{2} - \frac{\mathbf{R}+\mathbf{R}'}{2}\right), \tag{31}$$

then the HF term is given by:

$$W_{\alpha\beta}(\mathbf{r},\mathbf{r}') = \lim_{n\to\infty}\frac{V_n}{n^3}\delta(\mathbf{r}-\mathbf{r}')\sum_{\eta}\int d\mathbf{x}\times \left[\delta_{\alpha\beta}\sum_{\gamma} v_{\gamma\eta}(\mathbf{r},\mathbf{x})v^*_{\gamma\eta}(\mathbf{r}',\mathbf{x}) - v_{\alpha\eta}(\mathbf{r},\mathbf{x})v^*_{\beta\eta}(\mathbf{r}',\mathbf{x})\right], \tag{32}$$

from which, using Eq. (20), we obtain that the HF term is identically zero. Notice that the result of this derivation does not depend on whether the Fermi gas is free or confined. This result also shows that neglecting the HF term in the BdG equations, as usually done in the theoretical mean-field treatment of Fermi gases, is indeed a consistent choice.

Moreover, these results allow one to cancel out divergences in the self-consistent equations, e.g. in the pairing function, without ad-hoc renormalization procedures, and clarify the short-range nature of the potential in the sense of the limit to the δ function, and extend the calculations to finite densities.

To test the ability of this finite-radius approach to solve the divergence problem, we apply our scheme to the solution of the BdG equations for an homogeneous system of strongly interacting fermions at unitarity. The solution for ultracold atoms at unitarity using FCI requires a nontrivial renormalization procedure [8].

C. Scattering view of the Bogoliubov–de Gennes equations

In our approach, we rewrite the BdG equations at zero temperature in terms of the on-shell T-matrix and then perform our limit procedure, retaining Eq. (9) as a definition of the effective range of the interaction potential.

The equation for the pairing function Δ defined in Eq. (25) is readily seen to be

$$\Delta_{\alpha\beta}(\mathbf{r},\mathbf{r}') = -\int d\mathbf{R}d\mathbf{R}' \sum_{\alpha'\beta'} V_{\alpha\beta,\alpha'\beta'}(\mathbf{r},\mathbf{r}';\mathbf{R},\mathbf{R}')\times \sum_{\gamma}\int d\mathbf{x}\; u_{\alpha'\gamma}(\mathbf{R},\mathbf{x})v^*_{\beta'\gamma}(\mathbf{R}',\mathbf{x}) \equiv -V\mathcal{Q} \tag{33}$$

where in the last equality we have formally written the double integral as a "matrix product". In the case of the FCI potential, the equation as it stands plagued by a ultraviolet divergence.

Equation (33) can be rewritten using the Lippmann–Schwinger equation (11), so that the pairing function is determined by the normalized interaction (embodied in the T matrix) instead of the "bare" interaction described by the potential V[8].

This is achieved by rewriting the LS equation as $V = (1 - VG_0(E))T$ and considering the quantity $\Delta - VG_0(E)\Delta$. Using Eq. (33), we have the equalities

$$\Delta - VG_0\Delta = -V\mathcal{Q} - VG_0\Delta \tag{34}$$
$$= -V(\mathcal{Q} + G_0\Delta) \tag{35}$$
$$= -(1 - VG_0)T(\mathcal{Q} + G_0\Delta) \tag{36}$$

from which, assuming that $(1-VG_0(E))$ is invertible, we get

$$\Delta = -T(\mathcal{Q} + G_0(E)\Delta) \tag{37}$$

which is an equation for the pairing function involving the T matrix instead of the "bare" potential V. The solution of equation (37) has of course to be determined self consistently with the solution of the BdG equations (29). Introducing the indices α and β, denoting internal degrees of freedom of the atoms, Eq. (37) reads:

$$\Delta_{\alpha\beta,\mathbf{p}} = -\int\frac{d\mathbf{p}'}{(2\pi)^3}\sum_{\alpha'\beta'} T_{+;\alpha\beta,\alpha'\beta'}(E;\mathbf{p},\mathbf{p}')\times \left(\sum_q u_{\alpha' q,\mathbf{p}'}v^*_{\beta' q,\mathbf{p}'} + \frac{1}{E - E_{\alpha'} - E_{\beta'} - \frac{p'^2}{m}}\Delta_{\alpha'\beta',\mathbf{p}'}\right) \tag{38}$$

In the previous expression the value of the parameter E can be chosen arbitrarily and we have used this freedom to have a better convergence of the self-consistent solution.

III. AB-INITIO CALCULATION OF THE MULTICHANNEL T-MATRIX

We use Eq. (38) to study an ultracold gas of ^{6}Li atoms at unitarity [25], where the scattering length is infinite, and the observables, notably the pairing gap and the chemical potential, are proportional to the Fermi momentum of the free gas [1]. Such a regime can be obtained by exploiting the Feshbach resonance of a ^{6}Li spin-mixture. Experimental measurements [26, 27] show two Feshbach resonances for a magnetic strength of 543.28 G (narrow resonance) and $822\cdots834$ G (broad resonance), respectively.

The atom-atom collisions are described by an Hamiltonian of the form

$$H = T + H_{\rm el} + V_{\rm hf} + V_B, \tag{39}$$

where T is the kinetic energy of the nuclei, $H_{\rm el}$ is the electron Hamiltonian (including electronic kinetic energy, Coulomb potential and spin-orbit coupling), and $V_{\rm hf}$ is the hyperfine interaction. We have also included a term

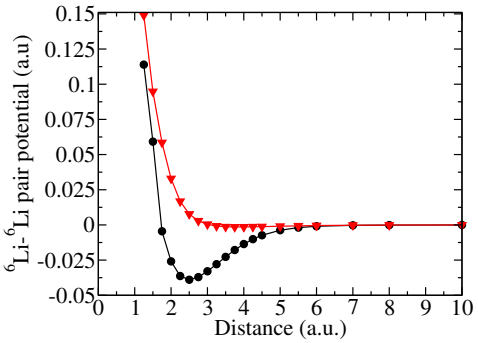

FIG. 1. PES for the singlet (dots) and triplet (triangles) states in ^{6}Li-^{6}Li scattering.

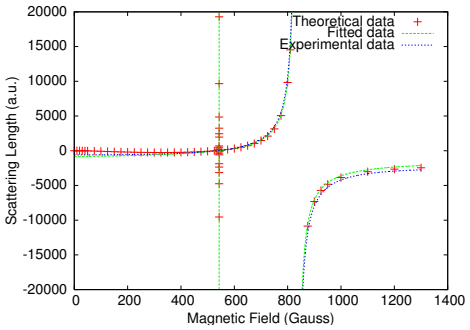

FIG. 2. S-wave scattering length vs applied magnetic field for the hyperspin states $(f, m_f\ ) = (1/2,\text{-}1/2)$ and $(1/2,\ 1/2)$ in ^{6}Li-^{6}Li scattering.

V_B describing the interaction of the atoms with an external magnetic field.

In the usual Born–Oppenheimer approximation, the wave equation for the relative motion of a pair of ultracold atoms at zero angular momentum can be written as

$$-\frac{\hbar^2}{2m}\nabla^2\phi_\alpha(r)+V_\alpha(r)\phi_\alpha(r)+\sum_\beta V_{I,\alpha\beta}(r)\phi_\beta(r) = E\phi_\alpha(r) \tag{40}$$

where the label α denotes the total electron and nuclear spin states of the colliding atoms. $V_\alpha(r)$ is the internuclear potential obtained using the ground-state electronic wavefunction for the given value of α, and $V_{I,\alpha\beta}(r)$ describes the coupling induced by the hyperfine interaction term, $V_{\rm hf}$, and the interaction with the magnetic field, V_B.

From the solution of Eq. (40) in the $E \to 0$ limit, one can obtain the s-wave scattering length a of the system from the asymptotic values of the wavefunction, that is

$$\phi_\alpha(r) = A_0\left(1-\frac{a}{r}\right). \tag{41}$$

In our theoretical analysis, the ^{6}Li-^{6}Li pair potentials appearing in Eq. (40) as a function of the external magnetic field have been calculated by using Configuration Interaction with single and double excitations from the reference Hartree–Fock ground state, taking into account fine and hyperfine structure terms [28]. Slater determinants have been built by expanding the molecular orbitals in a cc-pVQZ basis set of atomic-centered Gaussians. The electronic singlet and triplet potential energy surfaces are reported in Fig. 1 using dots and triangles, respectively.

In Fig. 2 we plot the calculated s-wave scattering length vs magnetic field for the lowest energy hyperspin doublet open channel. The positions of the narrow (543.25 G) and broad (834 G) resonances are in good agreement with the experimental data [27].

The T-matrix elements appearing in Eq. (38) have been computed by means of multichannel scattering theory [28]. To perform this calculation we have included relativistic terms (of the order of 2×10^{-6} a.u.), which mix the singlet and triplet states, and we have multiplied each of the *ab-initio* curves of the potential by a single parameter fixed to reproduce the values of the Feshbach resonances.

Since the open and closed channels are coupled via the hyperfine interaction, the problem is very complex if one takes into account the full on-shell multichannel T-matrix in the gap equation (38). Therefore, while the calculation of $T_+(0)$ has been performed in the multichannel space, we projected the T-matrix on the lowest hyperspin-doublet open channel to solve the BdG gap equation. This assumption is less drastic than using the interaction potential projected onto the open channel. In fact, the projected multichannel $T_+(0)$ matrix retains short range interactions with the closed channels and this is the reason why we prefer to use $T_+(0)$ rather than V in the self-consistent equation (38).

The on-shell $T_+(0)$ is represented over 10^5 equally spaced grid points, while a grid of 200×200 k-points according to a Gauss–Chebyshev quadrature over the interval [0,1] has been used in the momentum space, to obtain a convergence below 10^{-5} a.u. At unitarity, we find that the values of the effective range a_0, which is usually defined in term of the s-wave phase shift (see Eq. (7)) are -600 a.u. and 80 a.u for the narrow and broad resonances, respectively. The dependence of a_0 on the resonance position and its large negative value in the narrow resonance rule out a_0 as a measure of the effective range of the screened potential at unitarity.

On the other hand, by using Eq. (9) as a definition of the effective radius, we obtain for r_0 values of 26.5806 a.u. and 26.5756 a.u. for the narrow and broad resonance, respectively, with a difference of less than 0.02 %. We consider this result as a further indication that the definition of the effective range based on the small-momentum expansion of the T-matrix is reasonable and gives consistent results.

Our methodology provides directly the values of the

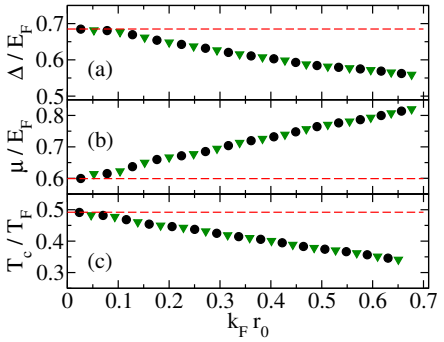

FIG. 3. Dimensionless gap function (a), chemical potential (b), and critical temperature (c) at unitarity for the narrow (dots), broad (triangles) resonances and for the δ-like interaction (dashed lines).

relevant quantities characterizing an ultra-cold Fermi gas – such as the gap, the chemical potential or the transition temperature – as a function of the effective range r_0. Their behavior is discussed in the following section.

IV. FINITE-RANGE EFFECTS IN THE UNITARY LIMIT FOR ^{6}LI

The ratios μ/E_F and Δ/E_F at unitarity as a function of $k_F r_0$ are plotted in the boxes (a) and (b) of Fig. 3, respectively. We observe that the behavior is exactly the same for the two resonances, as expected from the fact that we obtain the same value of the effective range for both the narrow and wide resonances.

These quantities are increasingly deviating from the curve of the δ-like interaction (dashed horizontal line) as the density is increased.

Using Quantum Monte Carlo (QMC) calculations, Gezerlis *et al.* [20, 29–31] obtained universal values at unitarity of $\Delta/E_f \approx 0.475 \pm 0.075$, $\mu/E_f \approx 0.4 \pm 0.075$, while Chang *et al.* [32] and Bulgac *et al.* [33] obtained $\Delta/E_f \approx 0.6 \pm 0.02$ and $\Delta/E_f \approx 0.58 \pm 0.02$, $\mu/E_f \approx 0.44 \pm 0.01$ and $\mu/E_f \approx 0.38 \pm 0.06$ respectively. It is not surprising that our calculations yield results that are consistently higher than those provided by QMC, since the BdG equations are based on a mean-field approximation of the fermion-fermion interaction. The BdG results are therefore very close to the BCS limit of $\Delta/E_f \approx 0.68$ and $\mu/E_f \approx 0.6$.

Although the derivation of the main equations of our approach has been carried out in the $T \to 0$ limit for the sake of conciseness, our theory can be straightforwardly extended to finite temperatures using Eq. (28). As a consequence, we can calculate the transition temperature T_c – defined as $\Delta(T_c) = 0$ – as a function of the parameter kr_0. This quantity, which is a very important parameter for any superfluid system, is reported in box (c) of Fig. 3. The ratio T_c/T_f has been previously estimated 0.494 at unitarity for a homogeneous system [34, 35]. Note that our theory predicts the same transition temperature at unitarity for both resonances, and it deviates up to 30 % of the corresponding FCI value by increasing the density of the system.

Our results show a significant density dependence for Δ, μ and T_c, in contrast with the predictions obtained using FCI for which a constant value is obtained for all these quantities. We estimate that the largest density that we have investigated (corresponding to $k_F r_0 = 0.6$) is about one order of magnitude larger than that achievable in modern harmonic traps [19]. Nevertheless, this value is likely reachable by experimental apparatus in a nearest future. At this high density, one might expect that three-body recombination could lead significant atom losses. However, we estimate that at equilibrium and for near threshold conditions 3-body recombination will play a little role even at such increased density regime, since the kinetic energy gain in the recombination process (10^{-17} a.u.) is very small compared to the Fermi energy (8×10^{-8} a.u.) [36].

V. CONCLUSIONS

To summarize, we have proposed a new definition of contact potential based on the the radius of the on-shell T-matrix at zero energy. This analysis underpins a short range, rather than a δ-like, model of the screened fermion-fermion interaction and rules out the scattering length and the usual effective radius as relevant parameters to describe dilute quantum gases at unitarity. Furthermore, we have shown the ability of our approach to cancel out naturally the divergences arising with the use of the contact potential. Finally, the application of this new theoretical approach to the self-consistent solution of the BdG equations for ultracold ^{6}Li homogeneous gas in the unitary regime has been discussed.

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